



A Robust Matrix-Free SQP Method for Large-Scale Optimization

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in collaboration with

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Intro & Outline

- *3rd talk on inexact SQP (F. Curtis, S. Ulbrich)!*
- optimal design, optimal control and inverse problems are often formulated as large-scale nonlinear programming problems (NLPs)
- can be solved, at least conceptually, using sequential quadratic programming (SQP) methods, **however ...**
- **inexactness in the iterative solution of linear systems** severely limits the effectiveness of conventional SQP algorithms for NLPs



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Inexact Trust-Region SQP
Heinkenschloss/R. (2006)

Inexact Line-Search SQP
Byrd/Curtis/Nocedal (2007)

Inexact Trust-Region SQP
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- overview of the 2010 algorithm for equality-constrained optimization
- application to a collection of PDE-constrained problems
- future work



Review of Trust-Region SQP

Solve NLP:

$$\begin{aligned} & \text{minimize} && f(x) \\ & \text{subject to} && c(x) = 0 \end{aligned}$$

where $f : \mathcal{X} \rightarrow \mathbb{R}$ and $c : \mathcal{X} \rightarrow \mathcal{C}$, for some Hilbert spaces \mathcal{X} and \mathcal{C} , and f and c are twice continuously Fréchet differentiable.

- define **Lagrangian functional** $\mathcal{L} : \mathcal{X} \times \mathcal{C} \rightarrow \mathbb{R}$:

$$\mathcal{L}(x, \lambda) = f(x) + \langle \lambda, c(x) \rangle_{\mathcal{C}}$$

- if *regular* point x_* is a local solution of the NLP, then there exists a $\lambda_* \in \mathcal{C}$ satisfying the **1st order necessary optimality conditions**:

$$\begin{aligned} \nabla_x f(x_*) + c_x(x_*)^* \lambda_* &= 0 \\ c(x_*) &= 0 \end{aligned}$$

- Newton's method applied to the 1st order optimality conditions:

$$\begin{pmatrix} \nabla_{xx}\mathcal{L}(x_k, \lambda_k) & c_x(x_k)^* \\ c_x(x_k) & 0 \end{pmatrix} \begin{pmatrix} s \\ z \end{pmatrix} = - \begin{pmatrix} \nabla_x f(x_k) + c_x(x_k)^* \lambda_k \\ c(x_k) \end{pmatrix}$$

- If $\nabla_{xx}\mathcal{L}(x_k, \lambda_k)$ is positive definite on the null space of $c_x(x_k)$, the above KKT system is necessary and sufficient for the solution of the QP:

$$\begin{array}{ll} \text{minimize} & \frac{1}{2} \langle \nabla_{xx}\mathcal{L}(x_k, \lambda_k) s, s \rangle_{\mathcal{X}} + \langle \nabla_x \mathcal{L}(x_k, \lambda_k), s \rangle_{\mathcal{X}} + \mathcal{L}(x_k, \lambda_k) \\ \text{subject to} & c_x(x_k) s + c(x_k) = 0 \end{array}$$

- To globalize convergence, we add a trust-region constraint:

$$\begin{array}{ll} \text{minimize} & \frac{1}{2} \langle H_k s, s \rangle_{\mathcal{X}} + \langle \nabla_x \mathcal{L}(x_k, \lambda_k), s \rangle_{\mathcal{X}} + \mathcal{L}(x_k, \lambda_k) \\ \text{subject to} & c_x(x_k) s + c(x_k) = 0 \\ & \|s\|_{\mathcal{X}} \leq \Delta_k \end{array}$$

→ note $H_k \approx \nabla_{xx}\mathcal{L}(x_k, \lambda_k)$

- Possible incompatibility of constraints: composite-step approach.

Composite-Step Approach for the Solution of the Quadratic Subproblem

- TR SQP step:

$$s_k = n_k + t_k$$

- quasi-normal step n_k :

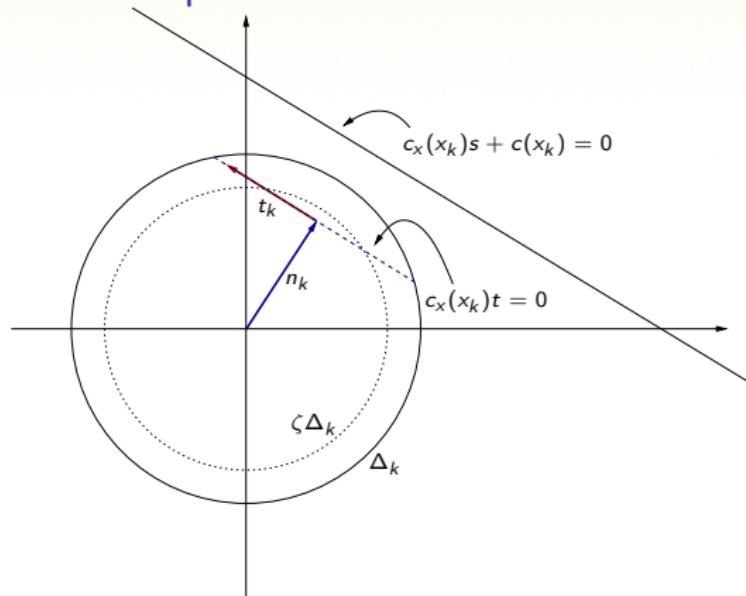
reduces linear infeasibility

$$\begin{array}{ll}\text{minimize} & \|c_x(x_k)n + c(x_k)\|_C^2 \\ \text{subject to} & \|n\|_{\mathcal{X}} \leq \zeta \Delta_k\end{array}$$

- tangential step t_k :

improves optimality while staying in the null space of the linearized constraints

$$\begin{array}{ll}\text{minimize} & \frac{1}{2} \langle H_k(t + n_k), t + n_k \rangle_{\mathcal{X}} + \langle \nabla_x \mathcal{L}(x_k, \lambda_k), t + n_k \rangle_{\mathcal{X}} + \mathcal{L}(x_k, \lambda_k) \\ \text{subject to} & c_x(x_k)t = 0 \\ & \|t + n_k\|_{\mathcal{X}} \leq \Delta_k\end{array}$$



e.g. Omojokun (1989), Byrd, Hribar, Nocedal (1997), Dennis, El-Alem, Maciel (1997)



Measuring Progress

- Lagrange multiplier estimate λ_{k+1} :

$$\lambda_{k+1} = \underset{\lambda}{\text{minimize}} \| \nabla f(x_k + s_k) + c_x(x_k + s_k)^* \lambda \|_{\mathcal{X}}^2,$$

computed by solving the *augmented system*:

$$\begin{pmatrix} I & c_x(x_k + s_k)^* \\ c_x(x_k + s_k) & 0 \end{pmatrix} \begin{pmatrix} z \\ \lambda_{k+1} \end{pmatrix} = \begin{pmatrix} -\nabla_x f(x_k + s_k) \\ 0 \end{pmatrix}$$

- Augmented Lagrangian merit function:

$$\phi(x, \lambda; \rho) = f(x) + \langle \lambda, c(x) \rangle_C + \rho \|c(x)\|_C^2 = \mathcal{L}(x, \lambda) + \rho \|c(x)\|_C^2$$

- Actual reduction at step k :

$$\text{ared}(s_k; \rho_k) = \phi(x_k, \lambda_k; \rho_k) - \phi(x_k + s_k, \lambda_{k+1}; \rho_k)$$

- Predicted reduction at step k :

$$\begin{aligned} \text{pred}(s_k; \rho_k) = & \phi(x_k, \lambda_k; \rho_k) - \left[\mathcal{L}(x_k, \lambda_k) + \langle \nabla_x \mathcal{L}(x_k, \lambda_k), s_k \rangle_{\mathcal{X}} + \frac{1}{2} \langle H_k s_k, s_k \rangle_{\mathcal{X}} \right. \\ & \left. + \langle \lambda_{k+1} - \lambda_k, c_x(x_k) s_k + c(x_k) \rangle_C + \rho_k \|c_x(x_k) s_k + c(x_k)\|_C^2 \right] \end{aligned}$$



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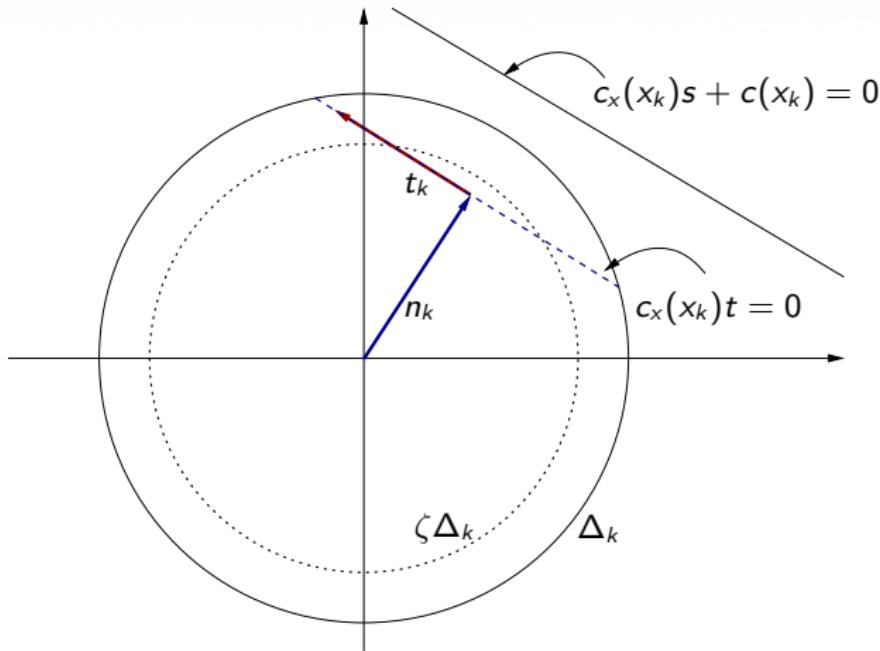
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because $c_x(x_k) t_k = 0$.

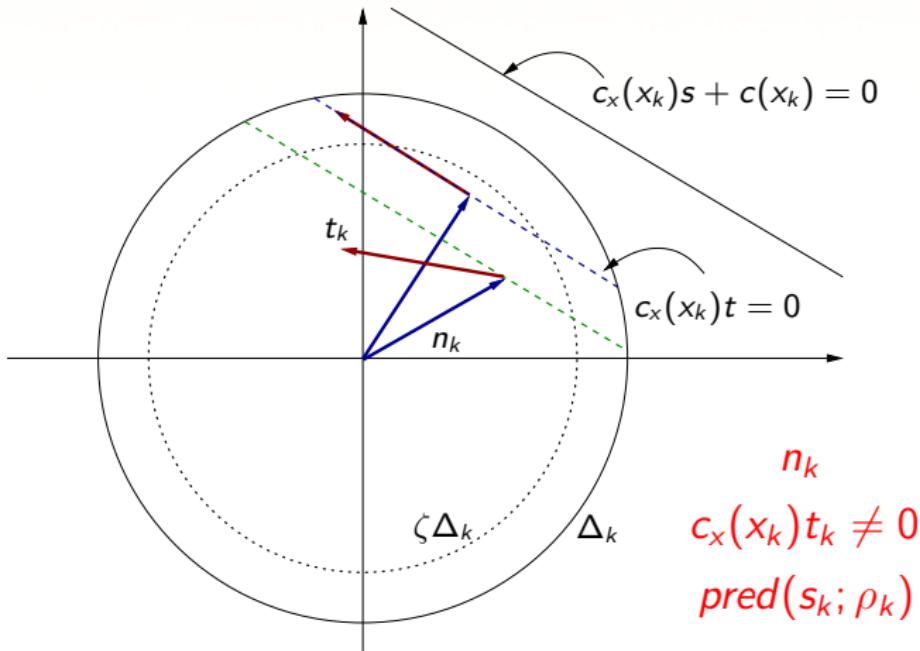


How to Throw a Wrench in the Trust-Region SQP Algorithm?





How to Throw a Wrench in the Trust-Region SQP Algorithm?





Inexact Quasi-Normal Step (2006)

GLOBAL CONVERGENCE CONDITIONS

The quasi-normal step n_k must satisfy the boundedness condition

$$\|n_k\|_{\mathcal{X}} \leq \kappa_1 \|c(x_k)\|_C,$$

and the sufficient decrease (s.d.) condition

$$\|c(x_k)\|_C^2 - \|c_x(x_k)n_k + c(x_k)\|_C^2 \geq \kappa_2 \|c(x_k)\|_C \min \{\kappa_3 \|c(x_k)\|_C, \Delta_k\},$$

where $\kappa_1, \kappa_2, \kappa_3 > 0$ are independent of k .

- Let n_k approximately solve the problem:

$$\begin{aligned} &\text{minimize} && \|c_x(x_k)n + c(x_k)\|_C^2 \\ &\text{subject to} && \|n\|_{\mathcal{X}} \leq \zeta \Delta_k. \end{aligned}$$

- A practical approach: Powell's dogleg method.

Inexact Quasi-Normal Step (2006)

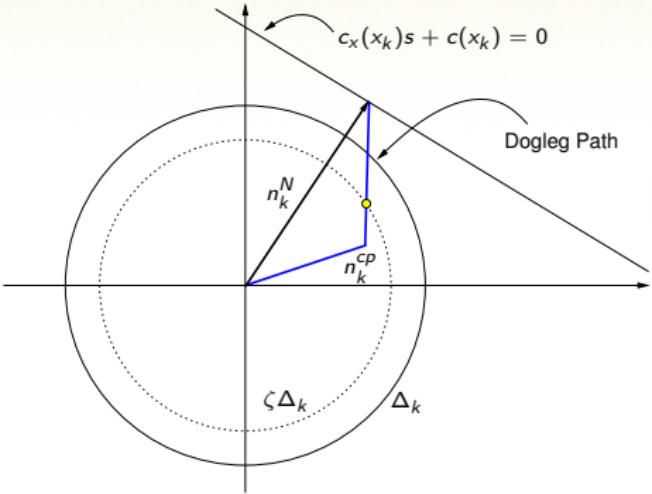
$$n_k^{cp} = \underset{\alpha \geq 0, \|n\|_{\mathcal{X}} \leq \zeta \Delta_k}{\text{minimize}} \quad \|c_x(x_k)n + c(x_k)\|_{\mathcal{C}}^2$$

subject to

$$n = -\alpha c_x(x_k)^* c(x_k)$$

n_k^N = minimum norm solution of

$$\underset{n}{\text{minimize}} \quad \|c_x(x_k)n + c(x_k)\|_{\mathcal{C}}^2$$



The minimum norm solution n_k^N can be computed by solving:

$$\begin{pmatrix} I & c_x(x_k)^* \\ c_x(x_k) & 0 \end{pmatrix} \begin{pmatrix} n_k^N \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ -c(x_k) \end{pmatrix}.$$

Inexact Quasi-Normal Step (2006)

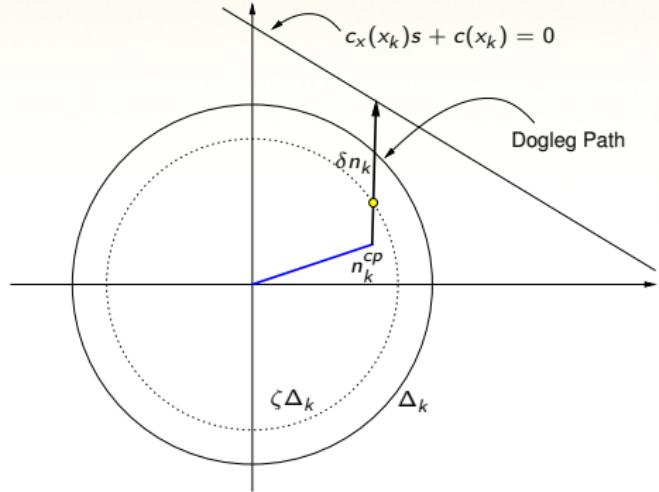
$$n_k^{cp} = \underset{\alpha \geq 0, \|n\|_{\mathcal{X}} \leq \zeta \Delta_k}{\text{minimize}} \quad \|c_x(x_k)n + c(x_k)\|_{\mathcal{C}}^2$$

subject to

$$n = -\alpha c_x(x_k)^* c(x_k)$$

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$$\underset{n}{\text{minimize}} \quad \|c_x(x_k)n + c(x_k)\|_{\mathcal{C}}^2$$



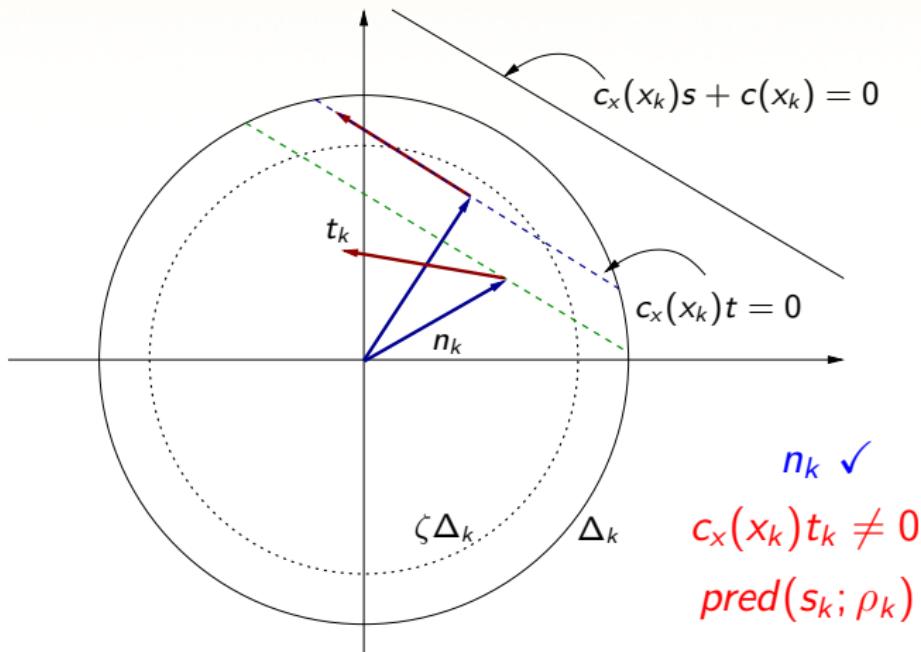
With inexactness, we solve for $\delta n_k = n_k^N - n_k^{cp}$:

$$\begin{pmatrix} I & c_x(x_k)^* \\ c_x(x_k) & 0 \end{pmatrix} \begin{pmatrix} \delta n_k \\ y \end{pmatrix} = \begin{pmatrix} -n_k^{cp} + r_k^1 \\ -c_x(x_k)n_k^{cp} - c(x_k) + r_k^2 \end{pmatrix}.$$

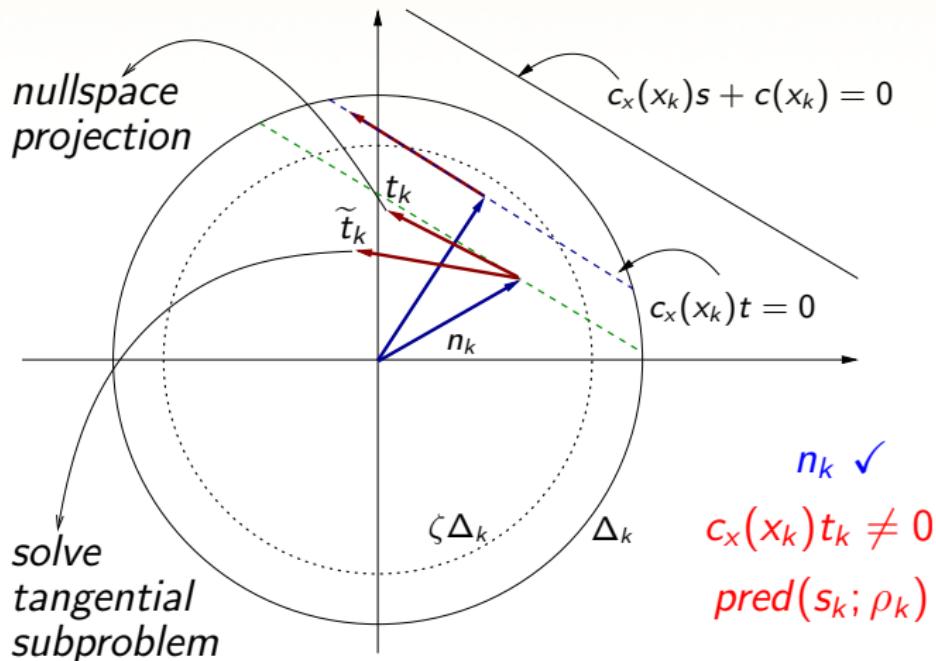
Theorem.

If $\|r_k^1\|_{\mathcal{X}}^2 + \|r_k^2\|_{\mathcal{C}}^2 \leq (C^{qn})^2 \|c_x(x_k)n_k^{cp} + c(x_k)\|_{\mathcal{C}}^2$, for a fixed $0 \leq C^{qn} \leq 1$, then the inexact quasi-normal step n_k satisfies boundedness and s.d. conditions.

Next: Inexact Tangential Step



Next: Inexact Tangential Step





Inexact Tangential Subproblem (2010)

..... Keep in mind: $t_k = \pi_k \tilde{t}_k$

- \tilde{t}_k approximately solves the tangential subproblem:

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \langle H_k(\tilde{t} + n_k), \tilde{t} + n_k \rangle_{\mathcal{X}} + \langle \nabla_x \mathcal{L}_k, \tilde{t} + n_k \rangle_{\mathcal{X}} + \mathcal{L}_k \\ & \text{subject to} && c_x(x_k) \tilde{t} = 0, \quad \|\tilde{t} + n_k\|_{\mathcal{X}} \leq \Delta_k. \end{aligned}$$

- Let $\Pi_k = \Pi_k^2$ be an exact null-space projector, use $g_k = H_k n_k + \nabla_x \mathcal{L}_k$:

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \langle H_k \tilde{t}, \tilde{t} \rangle_{\mathcal{X}} + \langle g_k, \tilde{t} \rangle_{\mathcal{X}} \\ & \text{subject to} && \tilde{t} \in \text{Range}(\Pi_k), \quad \|\tilde{t} + n_k\|_{\mathcal{X}} \leq \Delta_k. \end{aligned}$$

- Let $\tilde{\Pi}_k$ be the inexact null-space projector, reformulate:

$$\begin{aligned} & \text{minimize} && q_k(\tilde{t}) \equiv \frac{1}{2} \langle H_k \tilde{t}, \tilde{t} \rangle_{\mathcal{X}} + \langle \tilde{\Pi}_k g_k, \tilde{t} \rangle_{\mathcal{X}} \\ & \text{subject to} && \tilde{t} \in \text{Range}(\tilde{\Pi}_k), \quad \|\tilde{t} + n_k\|_{\mathcal{X}} \leq \Delta_k. \end{aligned}$$

Inexact Tangential Subproblem (2010)

GLOBAL CONVERGENCE CONDITIONS FOR TANGENTIAL SUBPROBLEM

The inexact reduced gradient $\tilde{\Pi}_k g_k$ must satisfy the accuracy condition

$$\|\tilde{\Pi}_k g_k - \Pi_k g_k\|_{\mathcal{X}} \leq \xi_1 \min \left(\|\tilde{\Pi}_k g_k\|_{\mathcal{X}}, \Delta_k \right);$$

the solution \tilde{t}_k of the tangential subproblem must satisfy the sufficient decrease (s.d.) condition

$$q_k(0) - q_k(\tilde{t}_k) \geq \kappa_4 \|\tilde{\Pi}_k g_k\|_{\mathcal{X}} \min \left\{ \kappa_5 \|\tilde{\Pi}_k g_k\|_{\mathcal{X}}, \kappa_6 \Delta_k \right\},$$

where $\xi_1, \kappa_4, \kappa_5, \kappa_6 > 0$ are independent of k .

Results

- Developed an **inexact CG with Steihaug-Toint stopping conditions**.
- Inexact projections $\tilde{\Pi}_k$ are applied by iteratively solving augmented systems. $\tilde{\Pi}_k$ can change at every CG iteration!
- The accuracy condition on the reduced gradient can be enforced explicitly.
- The algorithm ensures the sufficient decrease condition by construction.



Inexact Tangential Subproblem (2010)

Inexact Projected CG with Steihaug-Toint Stopping Conditions

- ① Given $\text{tol} > 0$. Let $\tilde{t}_{k,0} = 0 \in \mathcal{X}$. Let $\tilde{r}_0 = \tilde{\Pi}_k g_k$. If $\langle g_k, \tilde{r}_0 \rangle_{\mathcal{X}} = 0$, stop.
- ② For $i = 0, 1, 2, \dots, i_{\max}$
 - ③ If $i = 0$ set $\tilde{z}_0 = \tilde{r}_0$, else $\tilde{z}_i = \tilde{\Pi}_k \tilde{r}_i$. If $\|\tilde{z}_i\|_{\mathcal{X}} \leq \text{tol}$, return $\tilde{t}_{k,i}$.
 - ④ $\tilde{p}_i = -\tilde{z}_i + \sum_{j=0}^{i-1} \frac{\langle \tilde{z}_i, H_k \tilde{p}_j \rangle_{\mathcal{X}}}{\langle \tilde{p}_j, H_k \tilde{p}_j \rangle_{\mathcal{X}}} \tilde{p}_j$
 - ⑤ If $\langle \tilde{r}_i, \tilde{p}_i \rangle_{\mathcal{X}} \neq 0$ and $\langle \tilde{p}_i, H \tilde{p}_i \rangle_{\mathcal{X}} \leq 0$, compute θ such that $\text{sign}(\theta) = \text{sign}(-\langle \tilde{r}_i, \tilde{p}_i \rangle_{\mathcal{X}})$ and $\|n_k + \tilde{t}_{k,i} + \theta \tilde{p}_i\|_{\mathcal{X}} = \Delta_k$, and return $\tilde{t}_{k,i+1} = \tilde{t}_{k,i} + \theta \tilde{p}_i$.
If $\langle \tilde{r}_i, \tilde{p}_i \rangle_{\mathcal{X}} = 0$ and $\langle \tilde{p}_i, H \tilde{p}_i \rangle_{\mathcal{X}} < 0$, compute θ such that $\|n_k + \tilde{t}_{k,i} + \theta \tilde{p}_i\| = \Delta_k$, and return $\tilde{t}_{k,i+1} = \tilde{t}_{k,i} + \theta \tilde{p}_i$.
 - ⑥ If $\langle \tilde{r}_i, \tilde{p}_i \rangle_{\mathcal{X}} = 0$, return $\tilde{t}_{k,i}$.
 - ⑦ $\tilde{\alpha}_i = -\frac{\langle \tilde{r}_i, \tilde{p}_i \rangle_{\mathcal{X}}}{\langle \tilde{p}_i, H_k \tilde{p}_i \rangle_{\mathcal{X}}}$
 - ⑧ $\tilde{t}_{k,i+1} = \tilde{t}_{k,i} + \tilde{\alpha}_i \tilde{p}_i$
 - ⑨ If $\|n_k + \tilde{t}_{k,i+1}\|_{\mathcal{X}} \geq \Delta_k$, compute θ such that $\text{sign}(\theta) = \text{sign}(\tilde{\alpha}_i)$ and $\|n_k + \tilde{t}_{k,i} + \theta \tilde{p}_i\|_{\mathcal{X}} = \Delta_k$, and return $\tilde{t}_{k,i+1} = \tilde{t}_{k,i} + \theta \tilde{p}_i$.
 - ⑩ $\tilde{r}_{i+1} = H_k \tilde{t}_{k,i+1} + \tilde{\Pi}_k g_k = \tilde{r}_i + \tilde{\alpha}_i H_k \tilde{p}_i$



Tangential Step (2006)

$$t_k = \pi_k \tilde{t}_k$$

- The definition of predicted reduction follows Heinkenschloss/Vicente:

$$\widehat{\text{pred}}(s_k; \rho_k) \equiv \text{pred}(n_k, \tilde{t}_k; \rho_k) + r\text{pred}(r_k^t; \rho_k),$$

where $r_k^t \equiv c_x(x_k)t_k$.

- The accuracy of the final projection is governed by

$$|r\text{pred}(r_k^t; \rho_k)| \leq \eta_0 \text{pred}(n_k, \tilde{t}_k; \rho_k),$$

$$\|t_k - \pi_k \tilde{t}_k\|_{\mathcal{X}} \leq \xi_3 \Delta_k \min\{\Delta_k, \|s_k\|_{\mathcal{X}}\},$$

$$\|\tilde{t}_k\|_{\mathcal{X}} \leq \xi_4 \|s_k\|_{\mathcal{X}},$$

where $\eta_0 \in (0, 1 - \eta_1)$, and $\eta_1 \in (0, 1)$ is the smallest acceptable ratio of the actual and predicted reduction, and $\xi_3, \xi_4 > 0$ are independent of k .



A Collection of Medium-to-Large Scale PDE-Constrained Optimization Problems

Setup:

- Simple steady-state PDEs
- Discretize-then-optimize
- Linear finite element discretization
- Solver for augmented systems: GMRES (ILUT, 1,2-Level DD)
- SQP tolerance: 10^{-6} (feasibility and optimality)



Distributed Control of Burgers' Equation

Conventional Trust-Region SQP with Fixed Relative Tolerances

	1e-1	1e-2	1e-3	1e-4	1e-5	1e-6	1e-7	1e-8	1e-9	1e-10
GMRES	F	F	F	F	F	F	7054	6793	6763	4268
Avg./call	-	-	-	-	-	-	16.0	17.1	17.8	18.6
SQP	-	-	-	-	-	-	15	15	15	14
Nonconvex	-	-	-	-	-	-	7	7	7	7

Inexact Trust-Region SQP with A Simple Convergence “Knob”

	1e-1	1e-2	1e-3	1e-4	1e-5	1e-6	1e-7	1e-8	1e-9	1e-10
GMRES	9842	5914	4891	2792	2677	✓	✓	✓	✓	✓
Avg./call	10.2	12.4	13.9	14.8	15.4	✓	✓	✓	✓	✓
SQP	150	51	27	18	17	✓	✓	✓	✓	✓
Nonconvex	3	5	8	6	6	✓	✓	✓	✓	✓



Boundary Control of a Simplified 'Real' Ginzburg-Landau Equation

Conventional Trust-Region SQP with Fixed Relative Tolerances

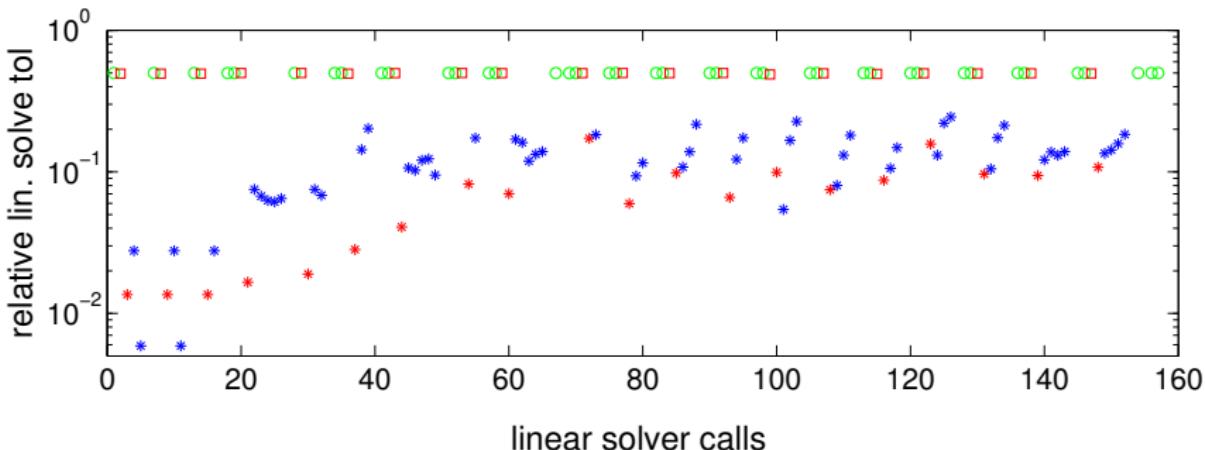
	1e-1	1e-2	1e-3	1e-4	1e-5	1e-6	1e-7	1e-8	1e-9	1e-10
GMRES	F	F	F	919	1013	1118	1205	1281	1354	1414
Avg./call	-	-	-	16.4	18.1	19.6	21.1	22.5	23.8	24.8
SQP	-	-	-	9	9	9	9	9	9	9
Nonconvex	-	-	-	6	6	6	6	6	6	6

Inexact Trust-Region SQP with A Simple Convergence "Knob"

	1e-1	1e-2	1e-3	1e-4	1e-5	1e-6	1e-7	1e-8	1e-9	1e-10
GMRES	1041	1051	1065	1176	1272	✓	✓	✓	✓	✓
Avg./call	11.4	13.6	15.4	17.0	18.4	✓	✓	✓	✓	✓
SQP	13	11	10	10	10	✓	✓	✓	✓	✓
Nonconvex	3	5	8	6	6	✓	✓	✓	✓	✓

Boundary Control of a Simplified 'Real' Ginzburg-Landau Equation

Turn the knob to **0.5**





Distributed Control of a Simplified Drift-Diffusion Semiconductor Model

Conventional Trust-Region SQP with Fixed Relative Tolerances

	1e-1	1e-2	1e-3	1e-4	1e-5	1e-6	1e-7	1e-8	1e-9	1e-10
GMRES	F	F	F	F	F	F	F	2008	2339	2653
Avg./call	-	-	-	-	-	-	-	9.9	11.6	13.1
SQP	-	-	-	-	-	-	-	20	20	20
Nonconvex	-	-	-	-	-	-	-	0	0	0

Inexact Trust-Region SQP with A Simple Convergence “Knob”

	1e-1	1e-2	1e-3	1e-4	1e-5	1e-6	1e-7	1e-8	1e-9	1e-10
GMRES	S	2269	2251	1199	1426	✓	✓	✓	✓	✓
Avg./call	-	3.8	5.0	5.9	7.6	✓	✓	✓	✓	✓
SQP	-	47	30	19	17	✓	✓	✓	✓	✓
Nonconvex	-	4	2	0	0	✓	✓	✓	✓	✓



Boundary Control of Navier-Stokes Equations

Conventional Trust-Region SQP with Fixed Relative Tolerances

	1e-1	1e-2	1e-3	1e-4	1e-5	1e-6	1e-7	1e-8	1e-9	1e-10
GMRES	F	F	F	F	F	F	3583	3988	4333	4666
Avg./call	-	-	-	-	-	-	19.9	22.4	24.3	26.4
SQP	-	-	-	-	-	-	8	8	8	8
Nonconvex	-	-	-	-	-	-	0	0	0	0

Inexact Trust-Region SQP with A Simple Convergence “Knob”

	1e-1	1e-2	1e-3	1e-4	1e-5	1e-6	1e-7	1e-8	1e-9	1e-10
GMRES	S	8156	4203	3334	3652	✓	✓	✓	✓	✓
Avg./call	-	6.7	10.5	14.6	17.4	✓	✓	✓	✓	✓
SQP	-	89	18	10	9	✓	✓	✓	✓	✓
Nonconvex	-	0	0	0	0	✓	✓	✓	✓	✓



Future Work

- the test suite will be expanded and open-sourced in [Trilinos](#) (as part of the [Aristos](#) optimization package of full-space methods, collaboration with Ross Bartlett, Sandia):
 - PDE discretizations ([Intrepid](#) library), linear solvers and preconditioners (for KKT systems: ILU and overlapping DD), AD, meshing and partitioning, parallel, ...
 - will provide a Matlab companion
 - September 2010
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- Byrd/Curtis/Nocedal vs. Heinkenschloss/R. comparison?
- most engineering problems are, eventually, inequality-constrained problems
 - next: [inexact interior-point trust-region methods](#)
- must be followed by advances in KKT preconditioning

